

Acetaldehyde

75-07-0 | DTXSID5039224

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 23.9 °C

Global applicability domain: Inside

Local applicability domain index: 6.16e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acetaldehyde</div> <div>Measured: 20.1</div> <div>Predicted: 23.9</div>	<div>Image not found</div> <div>Ethylene oxide</div> <div>Measured: 10.6</div> <div>Predicted: 11.9</div>	<div>Image not found</div> <div>Peroxide, dimethyl</div> <div>Measured: 14.0</div> <div>Predicted: 18.4</div>
<div>Image not found</div> <div>Acetone</div> <div>Measured: 55.8</div> <div>Predicted: 48.2</div>	<div>Image not found</div> <div>(2H6)Acetone</div> <div>Measured: 55.8</div> <div>Predicted: 50.0</div>	<div>Image not found</div> <div>Propanal</div> <div>Measured: 48.0</div> <div>Predicted: 47.1</div>